

Stereodynamics of some pyridoxine derivatives

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Abstract

Copyright © 2016 John Wiley & Sons, Ltd. The conformational properties of three pyridoxine derivatives were studied by ¹H dynamic NMR spectroscopy. Conformational exchange caused by a rotation of 2-nitrophenyl group around one single C-C bond, of 2,4-dinitrophenyl substituent around two single C-O bonds, and twist-twist transformations of the seven-membered ketal cycle was observed by NMR experiments at low temperatures. Meanwhile, the conformational exchange of the acetal ring remains fast in the NMR timescale even at 198 K. The energy barriers for all observed conformational exchange processes were determined by the lineshape analysis of dynamic NMR spectra. The activation barriers of the 2-nitrophenyl group rotation were almost the same for all studied compounds, about 40–41 kJ/mol. The energy barriers of the conformational exchange processes of the 2,4-nitrophenyl group and the ketal cycle increased significantly up to 10 kJ/mol in comparison with previously studied compounds with similar structure. Copyright © 2016 John Wiley & Sons, Ltd.

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Keywords

2D NOESY NMR, conformational exchange, dynamic ¹H NMR, energy barrier, pyridoxine

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